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January 23, 2024

Workshop: The building blocks of (nearly) everything: Using computational chemistry to study R&D dynamics

Preliminary Program

Event Date: February 15th-16th, 2024

Location: ESMT Berlin, Schlossplatz 1, 10178 Berlin, Germany, www.esmt.org.

Online participation: Online participation is possible via Zoom. Please register at <https://esmt-berlin.zoom.us/meeting/register/u5Aud-uhqT8uE9RDnKbSo301z9Odbo15-eyN>.

Organizers: Arianna Martinelli (Sant'Anna), Elisa Giuliani (University of Pisa), Stefan Wagner (ESMT Berlin)

Background:

Chemical compounds, often not found in nature, underpin a range of consumer goods from pharmaceuticals and cosmetics to industrial solvents, fertilizers, and pesticides. Despite their prevalence, knowledge gaps persist in our understanding of the R&D trajectories that give rise to such synthetic compounds, and their subsequent societal and environmental impacts.

This workshop spotlights the innovative application of computational chemistry in dissecting R&D dynamics, particularly emphasizing the use of chemical compound information in the pharma and chemistry domains. The focus is on understanding how computational methods can be synergized with traditional data sources like patents to provide deeper insights into R&D activities.

The second day of the workshop serves as an internal meeting of the working group of the organizers.

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Accommodation:

We recommend [ARCOTEL John F Berlin](#), which is within walking distance of ESMT Berlin.

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Schedule:

DAY 1 – 15th of February 2024

Time	Title	Presenter
9.30 – 10.00	Arrival and registration	
10.00 – 10.15	Welcome and overview	Organizers
10.15 – 10.50	Competition and Innovation: The Breakup of IG Farben	Felix Poege (Bocconi)
10.50 – 11.25	Shelved Innovation – Evidence from the Pharmaceutical Industry	Elisabeth Hofmeister (MPI)
11.25 – 12.10	Environmental Transparency and Value Appropriation from Innovation: Unpacking Trade Secrets in US Hydraulic Fracturing Chemical Disclosures	Shirley Tang (Bocconi)
12.10 – 13.10	Lunch break (ESMT canteen)	
13.15 – 13.50	International Environmental Agreements, and the Timing and Direction of Technological Change: Evidence from the Kigali Amendment	Albert Roger (MPI)
13.50 – 14.25	Are we moving to a less toxic world? How bans on Persistent Organic Pollutants affect firms' inventive strategies	Gianluca Biggi (School of Advanced Studies Sant'Anna)
14.25 – 15.10	Exploring Patterns of Pharmaceutical Post-Marketing Withdrawal	Nate Niu (ESMT)
15.10 – 15.45	Coffee break	
15.45 – 16.20	Exploring the dark side of firms' innovation: the role of the patent inventors' team	Vittoria Scalera (Amsterdam Business School)
16.20 – 17.00	Chemical Toxicity: Big Data Analysis and In Silico Predictions (Keynote speech)	Giulio Poli (University of Pisa)
17.15 – 17.45	Short tour of ESMT's historic campus	

19.30	Dinner and farewell Restaurant acht & dreissig https://restaurant38berlin.de/ https://maps.app.goo.gl/QoZVaCRBoLuEPDqT8	

DAY 2 – 16th of February 2024

Time	Title	Presenter
9.00 – 10.30	Workshop I	
10.30 – 11.00	Coffee break	
11.00 – 12.30	Workshop II	
12.30 – 13.30	Lunch and farewell (ESMT canteen)	

List of confirmed participants:

Gianluca Biggi

Post-doctoral Researcher in Economic Policy, Scuola Superiore Sant'Anna, Pisa

Sungyong Chang

Assistant Professor in Management, London Business School

Elisa Giuliani

Professor of Management, University of Pisa

Elisabeth Hofmeister

Doctoral Researcher in Economics of Innovation, MPI Munich

Arianna Martinelli

Associate Professor of Applied Economics, Scuola Superiore Sant'Anna, Pisa

Julia Mazzei

Post-doctoral Researcher in Applied Economics, Scuola Superiore Sant'Anna, Pisa

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Doctoral Researcher in Economics of Innovation, ESMT Berlin

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Post-doctoral Researcher in Economics of Innovation, ESMT Berlin

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Assistant Professor in Management and Technology, Bocconi

Giulio Poli

Post-doctoral Researcher in pharmaceutical chemistry, University of Pisa

Albert Roger

Post-doctoral Researcher in Economics of Innovation, MPI Munich

Vittoria Scalera

Associate Professor of International Business, Amsterdam Business School

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